

Supporting Information

An Energy-Dense and Thermal-Stable *bis*-Azobenzene/Hybrid

Templated Assembly for Solar Thermal Fuel

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Fig. S1 Dispersion of *bis-Azo* (10.3 mg L^{-1}) and *RGO-bis-Azo* (35.2 mg L^{-1}) in DMF. Dilute dispersions of *bis-Azo* (left) and *RGO-bis-Azo* (right) are used for photoisomerization measurements.

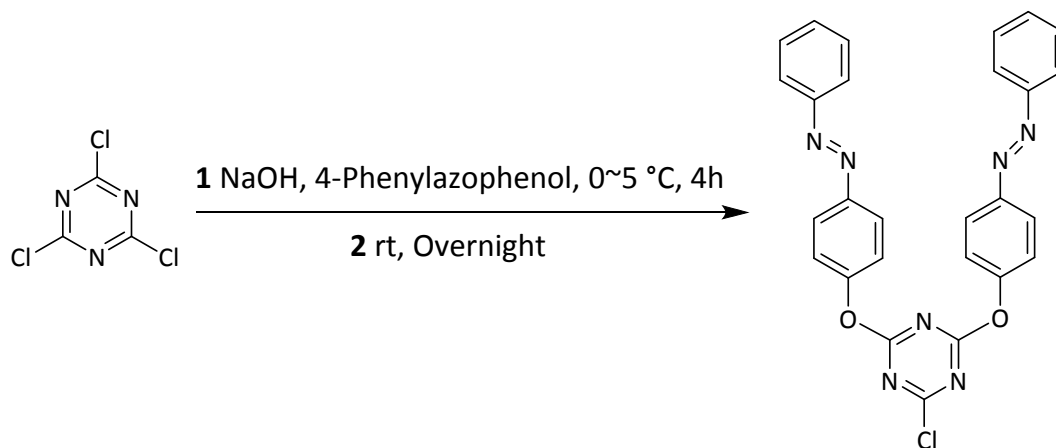


Fig. S2 Synthetic route of *bis-Azo*.

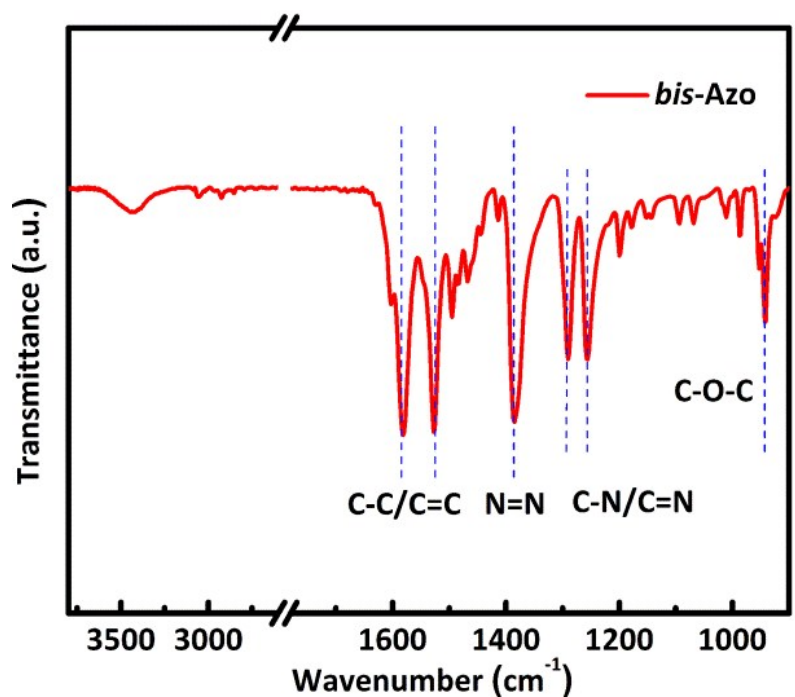


Fig. S3 FT-IR spectra of *bis-Azo*.

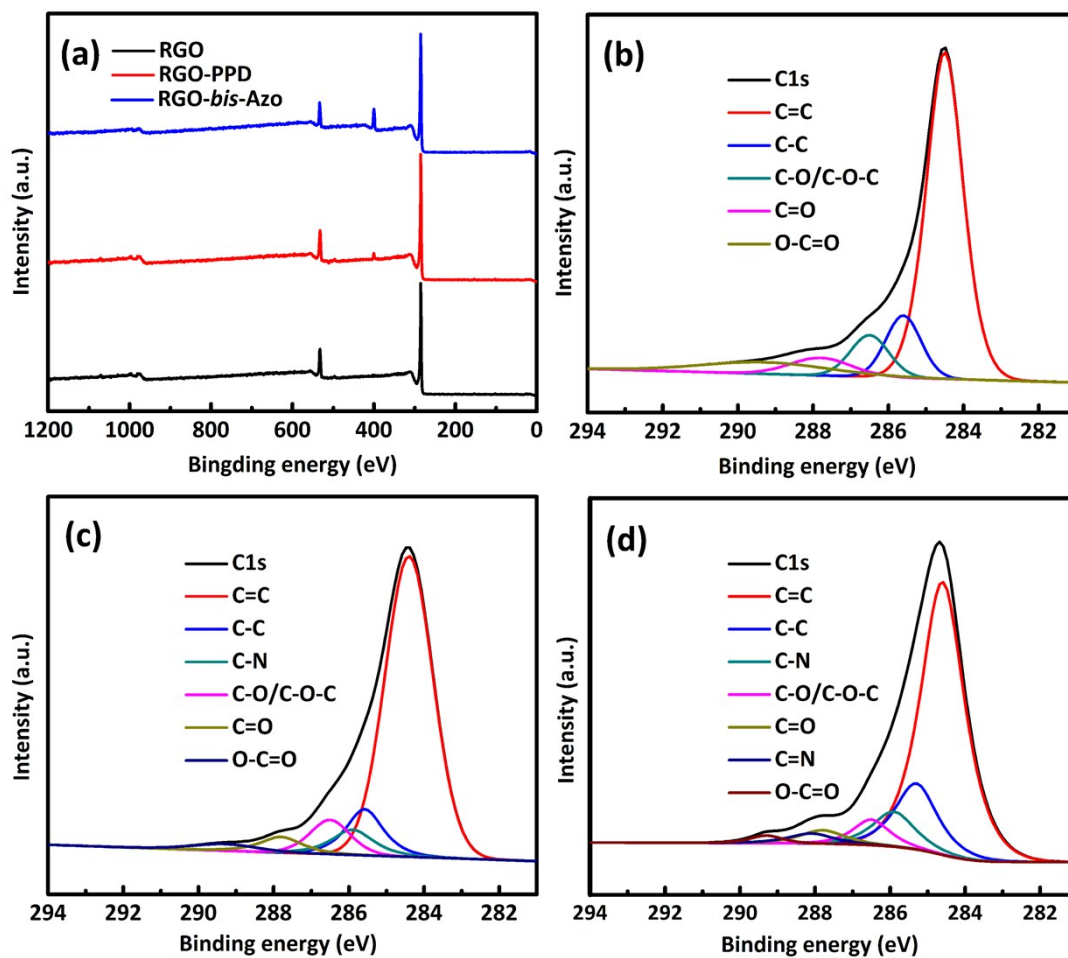


Fig. S4 (a) XPS wide scan survey spectra of RGO, RGO-PPD and RGO-*bis*-Azo. C1 region in XPS spectra of (b) RGO, (c) RGO-PPD and (d) RGO-*bis*-Azo.

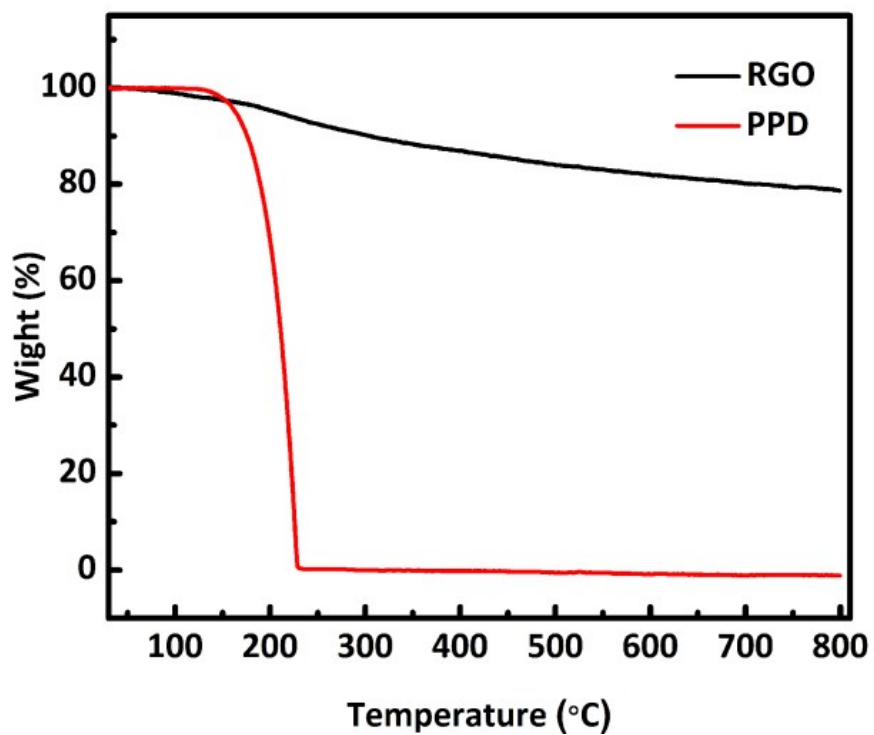


Fig. S5 TG curves of RGO and PPD.

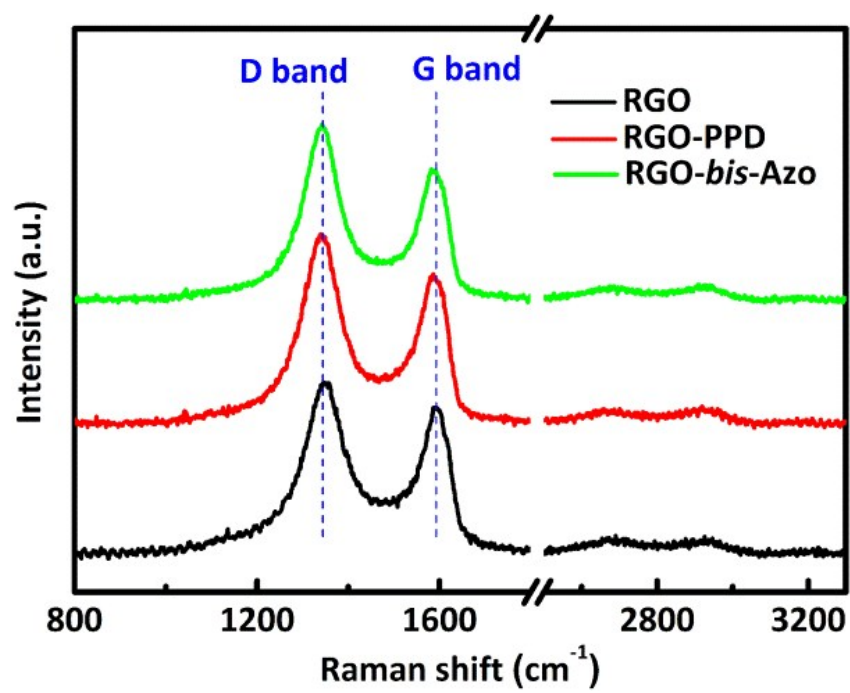


Fig. S6 Raman spectra of RGO, RGO-PPD and RGO-*bis*-Azo.

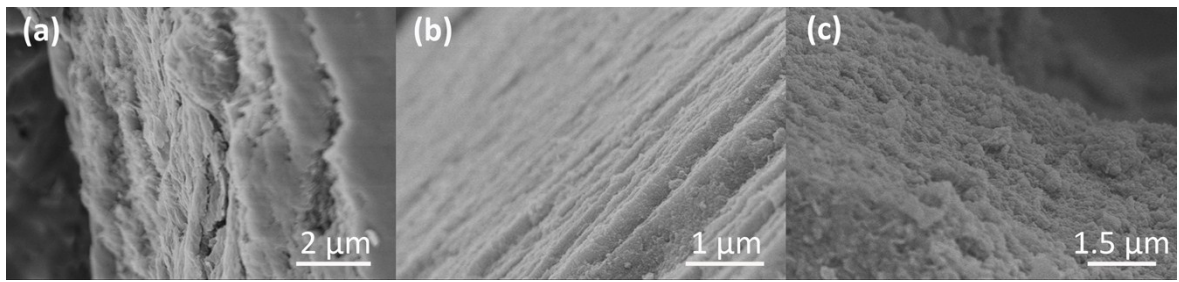


Fig. S7 SEM images of (a) RGO, (b) RGO-PPD and (c) RGO-*bis*-Azo.

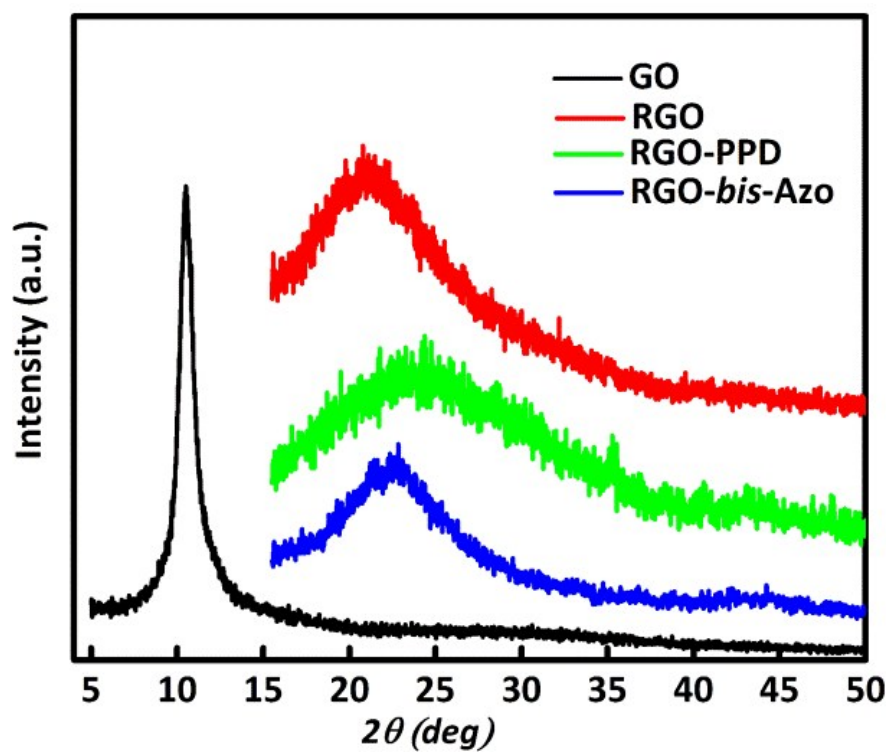


Fig. S8 XRD patterns of GO, RGO, RGO-PPD and RGO-*bis*-Azo.

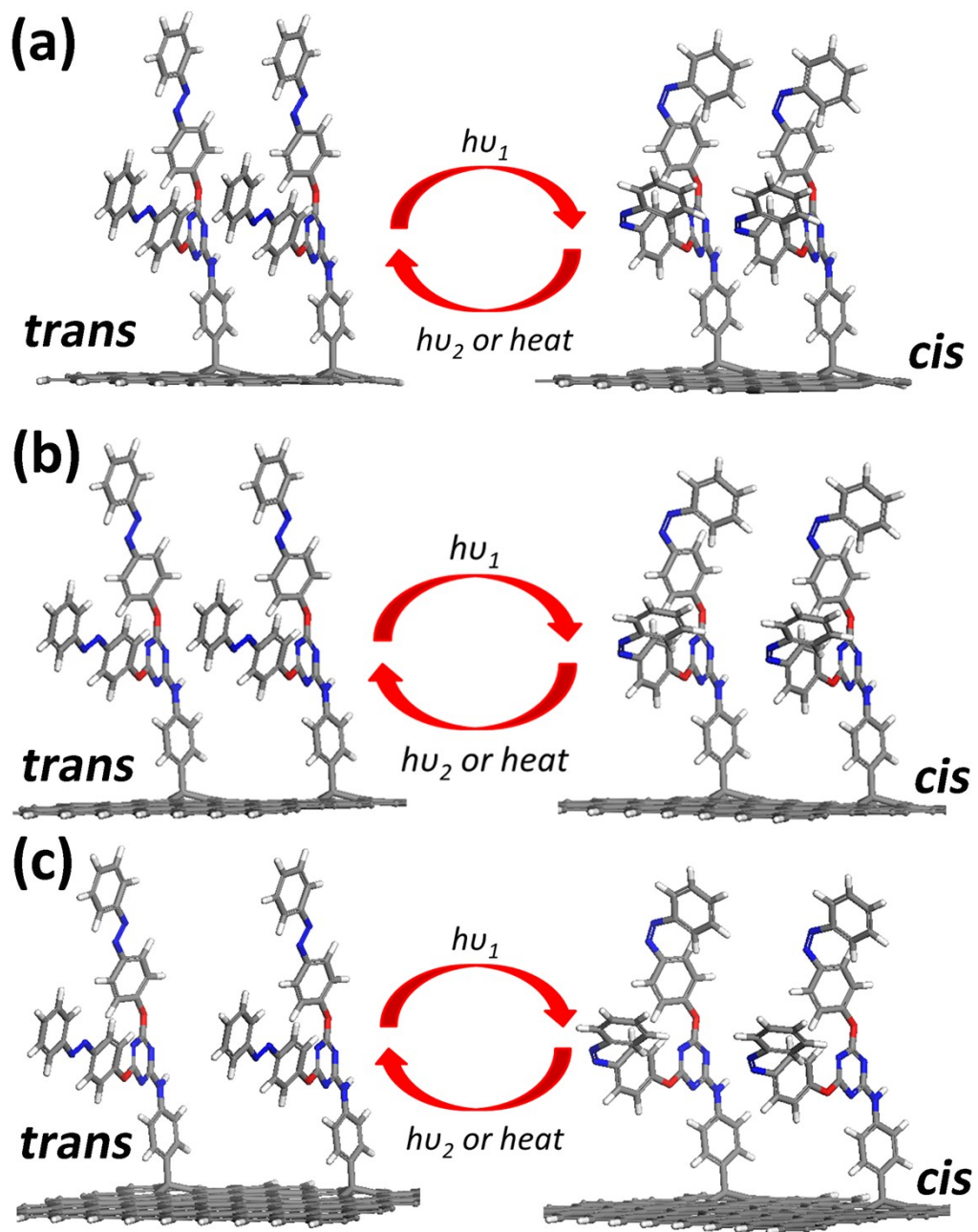


Fig. S9 Stable models of *trans*-isomer and *cis*-isomer by DFT calculation: (a) RGO-*bis*-Azo (1:54); (b) RGO-*bis*-Azo** (1:72); (c) RGO-*bis*-Azo* (1:90).

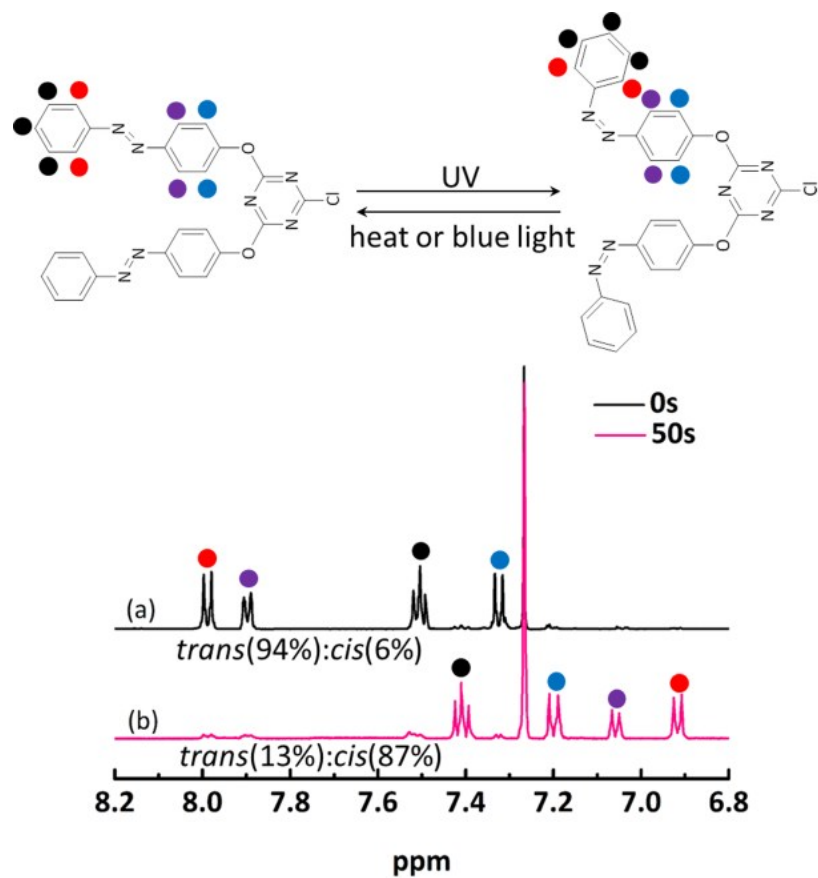


Fig. S10 $^1\text{H NMR}$ spectra of *bis*-Azo in CDCl_3 : (a) before the irradiation and (b) after UV irradiation for 50 s.

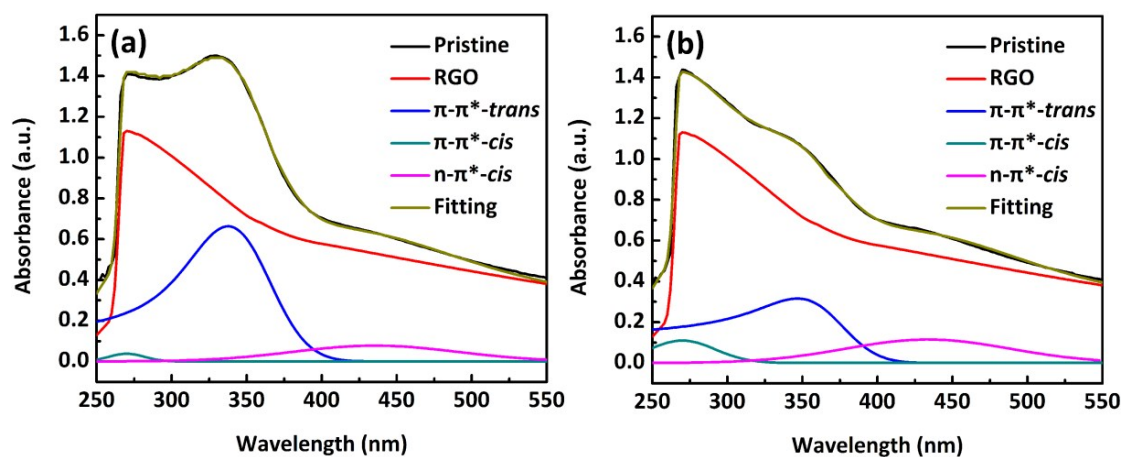


Fig. S11 The fitted absorption spectra of RGO-*bis*-Azo: (a) before the irradiation and (b) after UV irradiation for 130 min (at the photostationary state).

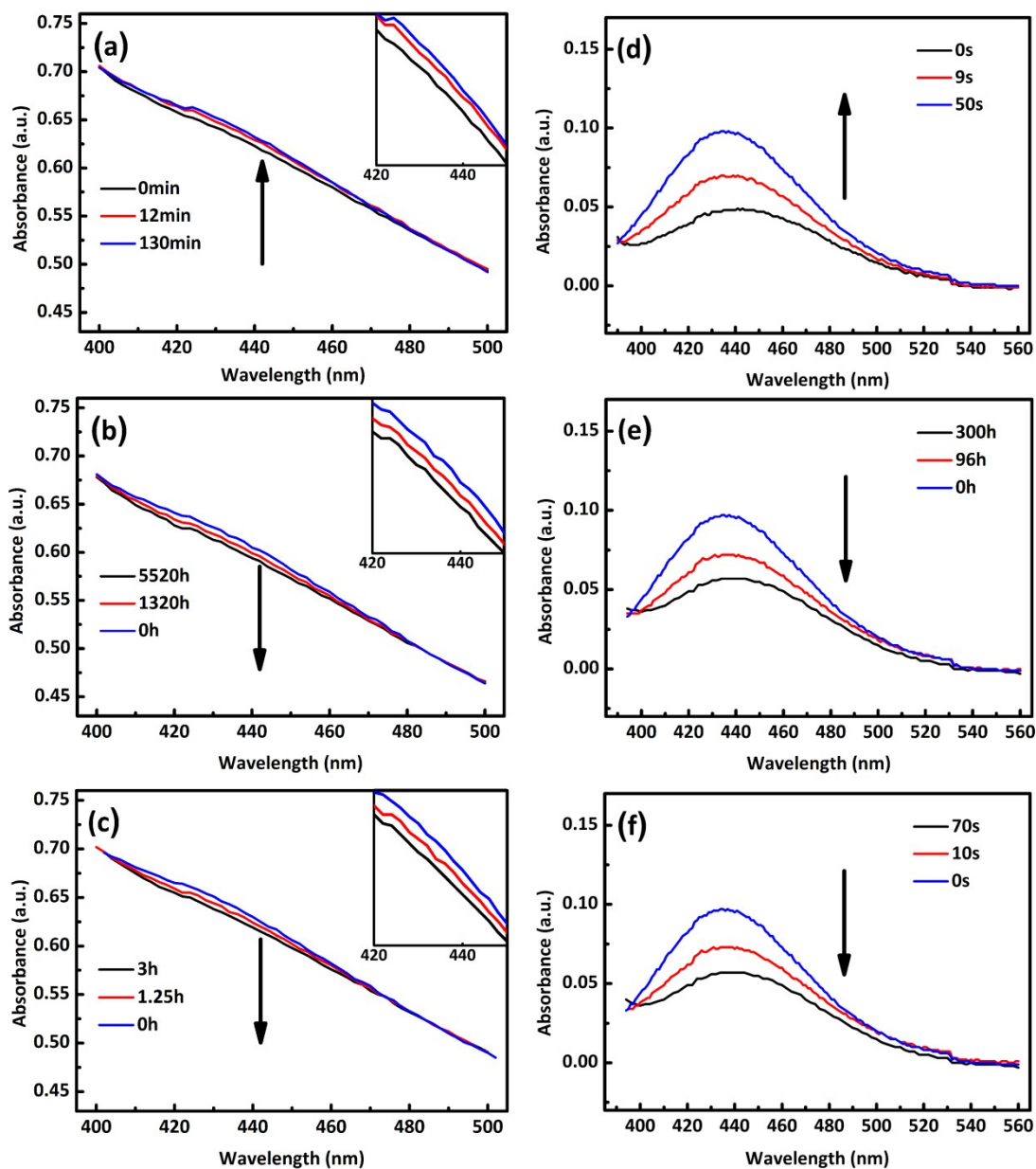


Fig. S12 Time-evolved absorption spectra for $n\text{-}\pi^*$ of RGO-*bis*-Azo (35.2 mg L⁻¹) and *bis*-Azo (10.3 mg L⁻¹) irradiated by (a, d) UV light at 365 nm, (b, e) after UV irradiation in darkness and (c, f) blue light at 450 nm.

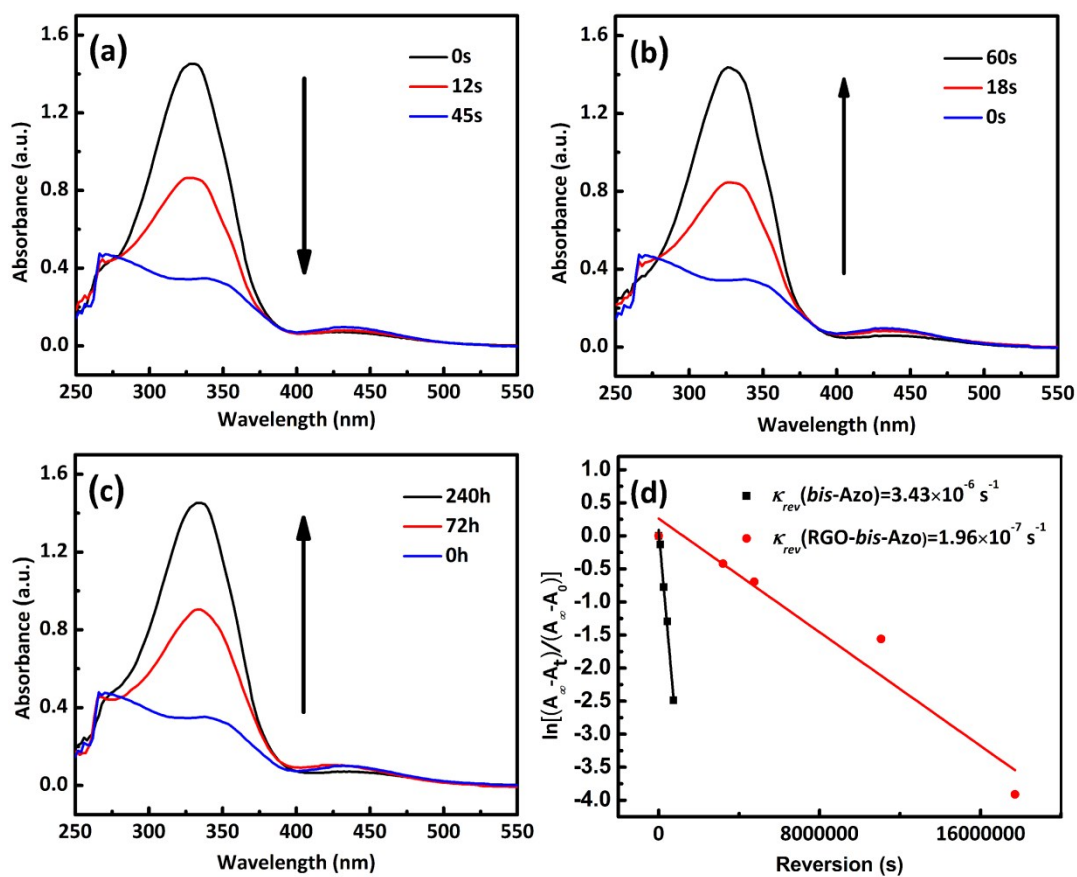


Fig. S13 Time-evolved absorption spectra of Azo (14.3 mg L^{-1}) changed at room temperature. (a) Azo irradiated by UV light at 365 nm, (b) Azo irradiated by blue light at 450 nm, (c) Azo reversed in darkness. (d) First plots of $cis \leftrightarrow trans$ reversion of RGO-*bis*-Azo and *bis*-Azo in darkness.

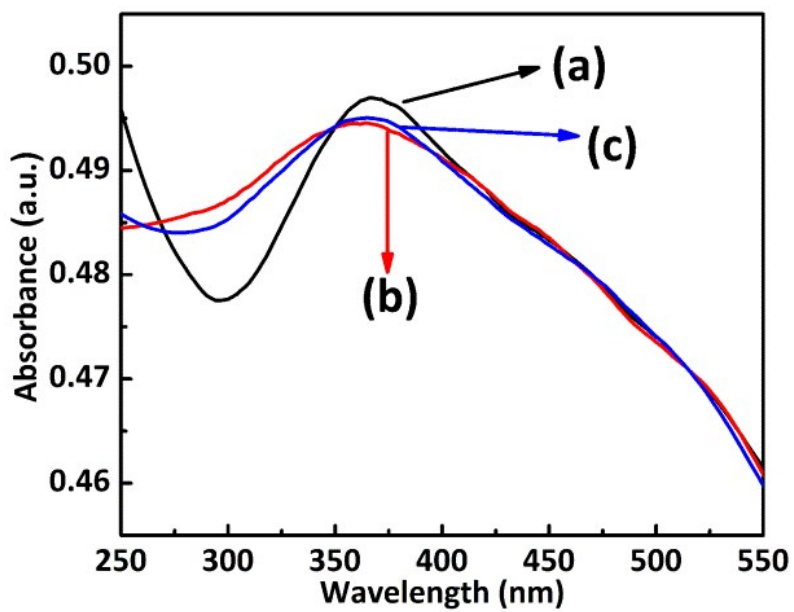


Fig. S14 Time-evolved absorption spectra of RGO-*bis*-Azo film (a) before the irradiation, (b) after UV irradiation for 2.5 h and (c) in dark for 840 h.

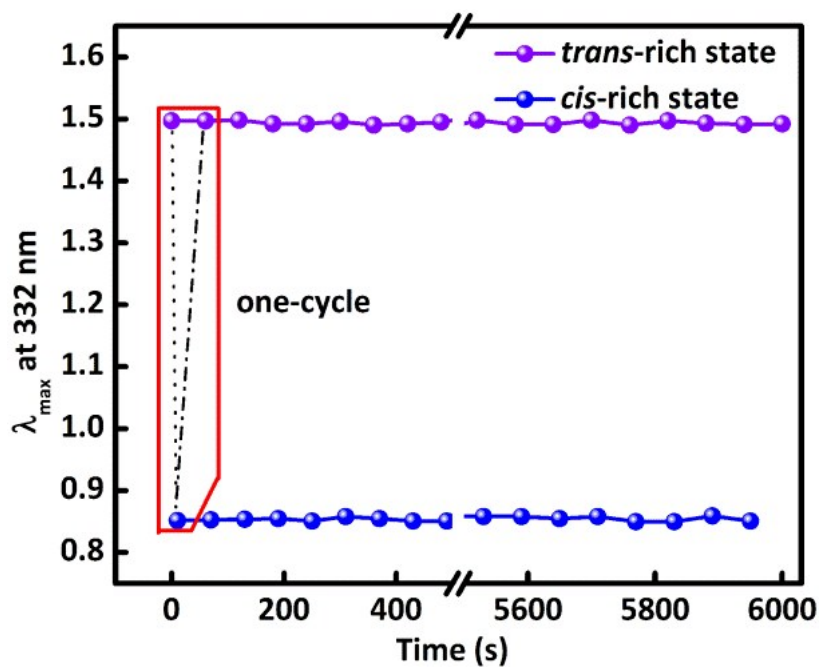


Fig. S15 Cycling stability of *trans* \leftrightarrow *cis* isomerization of *bis*-Azo in DMF induced by alternately irradiating UV light and blue light (450 nm) for 10 s and 50 s (at the photo-stationary balance). *bis*-Azo hybrid shows excellent cycling stability of *trans* \leftrightarrow *cis* isomerization for 100 cycles without degradation.

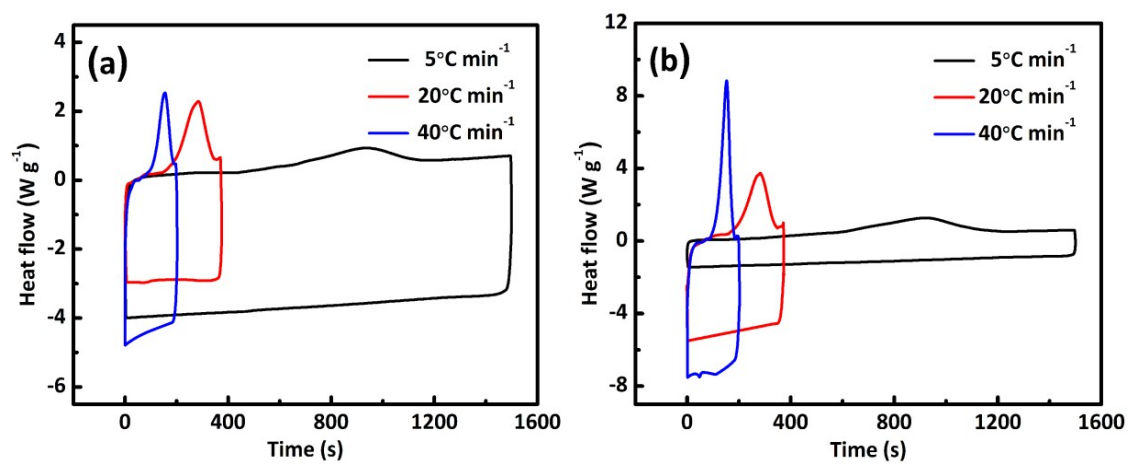


Fig. S16 DSC traces of (a) *bis*-Azo and (b) RGO-*bis*-Azo with different heating rates.

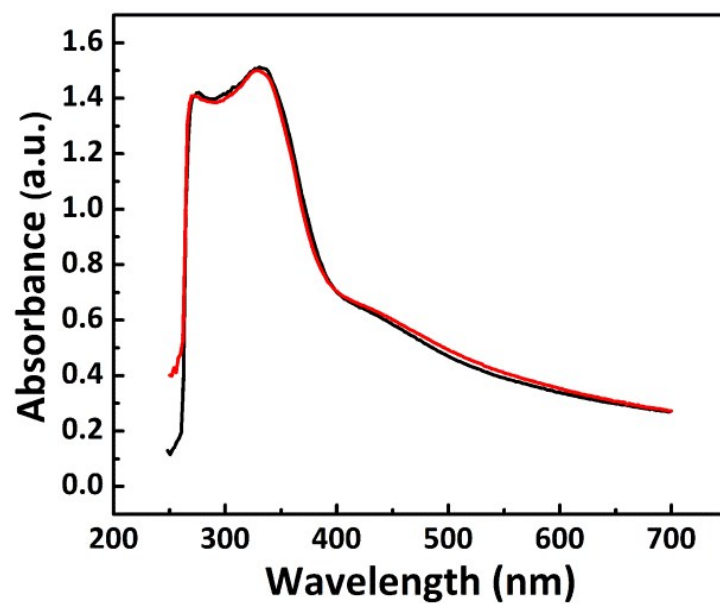


Fig. S17 Absorption spectra of RGO-*bis*-Azo in DMF before the irradiation (red) and after the first time heating (black) in DSC measurement.

Table S1. TGA and XPS data of RGO-*bis*-Azo.

	TGA			D_f	XPS		D_f
	700	D_t (%)			Element Content (%)		
		750	800		C	N	
RGO	81.92	81.14	79.55	/	85.1	/	
<i>bis</i> -Azo	29.39	25.65	21.87	/	/	/	
RGO-PPD	68.58	65.13	62.32	1:22.3	83.6	3.2	1:21
RGO- <i>bis</i> -Azo	57.06	52.20	49.18	1:51.1	79.2	10.1	1:50
RGO- <i>bis</i> -Azo*	67.95	64.70	61.87	1:91.2	81.3	7.6	1:91
RGO- <i>bis</i> -Azo**	68.10	64.50	61.85	1:73.5	80.6	8.4	1:74

D_f is grafting density; RGO-*bis*-Azo* and RGO-*bis*-Azo** are the hybrid with different grafting densities.

Table S2. Intensity ratio of D band to G band

	RGO	RGO-PPD	RGO- <i>bis</i> -Azo
I_D/I_G	1.14	1.27	1.30

Equation S1

$$D_f(\%) = \frac{R_p - R}{R_p - R_a} \times 100\%$$

R_a is the residual weight percentage of *bis*-Azo, R is the residual weight percentage of RGO-*bis*-Azo, R_p is the residual weight percentage of RGO-PPD.

Equation S2

$$\ln\left(\frac{A_\infty - A_t}{A_\infty - A_0}\right) = -k_{rev}t$$

A_0 is the absorption intensity of *bis*-Azo and RGO-*bis*-Azo at metastable state (*cis*-rich) irradiated by UV light, A_t is the absorption intensity of *bis*-Azo and RGO-*bis*-Azo reversing for “ t ” time and A_∞ is the absorption intensity of *bis*-Azo and RGO-*bis*-Azo after complete *cis*-trans reversion.

Equation S3

$$E_a = -RT \ln \frac{h \ln 2}{\tau_{1/2} k_B T}$$

T is the storage temperature and, $\tau_{1/2}$ is the half life. k_B , R and h are the Boltzman, gas and Plank constants, respectively.

Data S1. The coordinates of optimized Geometries for RGO-*bis*-AZO hybrids by DFT.

cis-RGO-*bis*-AZO (1:54)

C	0.665823837	10.476456136	1.700000000
C	0.665823837	13.317018214	1.700000000
C	0.665823837	14.737299253	1.700000000
C	0.665823837	17.577861331	1.700000000
C	0.665823837	18.998142369	1.700000000
C	0.665823837	21.838704447	1.700000000
C	0.665823837	23.258985486	1.700000000
C	0.665823837	26.099547564	1.700000000
C	0.665823837	27.519828603	1.700000000
C	6.835824377	11.186596656	1.700000000
C	5.605824917	10.476456136	1.700000000
C	4.375825457	11.186596656	1.700000000
C	6.835824377	12.606877694	1.700000000
C	5.605824917	13.317018214	1.700000000
C	6.835824377	15.447439772	1.700000000
C	3.145825997	10.476456136	1.700000000
C	1.915826536	11.186596656	1.700000000
C	4.375825457	12.606877694	1.700000000
C	3.145825997	13.317018214	1.700000000
C	5.605824917	14.737299253	1.700000000
C	4.375825457	15.447439772	1.700000000
C	6.835824377	16.867720811	1.700000000
C	5.605824917	17.577861331	1.700000000
C	6.835824377	19.708282889	1.700000000
C	1.915826536	12.606877694	1.700000000
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trans-RGO-*bis*-AZO (1:54)

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O	4.146779517	21.003520544	8.527160990
H	0.609624773	9.395700232	1.341658957
H	3.321582339	9.386048343	1.417651779
H	5.596286727	9.354936170	1.495789437
H	6.735469197	29.365473777	1.687430847
H	4.408457668	29.363811046	1.586256432
H	1.879097310	29.363685724	1.586256432
H	4.013449517	26.377660138	7.952205985
H	4.940119517	18.345378080	12.236297756
H	3.576979517	18.789132691	7.466170218
H	3.640409517	16.525332422	8.560236665
H	4.900499517	20.602166277	11.152381075
H	3.103199517	20.363488939	14.309727833
H	4.681659517	25.079015121	14.131795560
H	4.726149517	23.814042560	16.305617231
H	3.023069517	21.623135773	12.153627766
H	3.926199517	23.242803669	5.900850703
H	4.380529517	27.522488500	6.021661313
H	4.536779517	27.588733203	3.569988351
H	4.095819517	23.294131698	3.486238843
H	4.089609517	18.355960639	21.800008231
H	3.758219517	19.018034541	17.543427112
H	3.641439517	17.476040301	19.496522885
H	4.640419517	20.764566148	22.121387374
H	4.762299517	22.282165144	20.142218571
H	4.378739517	10.680384903	13.611358451
H	4.623129517	14.979797723	13.256961345
H	4.779649517	12.921807777	14.655278005
H	3.835429517	10.519928225	11.187810842
H	3.679469517	12.600354191	9.812104794

cis-RGO-*bis*-AZO** (1:72)

C	0.70204	10.50564	1.63250
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C	0.70138	13.33155	1.71136
C	0.70051	14.76103	1.72052
C	0.70043	17.60893	1.64920
C	0.69950	19.03608	1.57194
C	0.70066	21.88413	1.42491
C	0.70447	23.31464	1.40347
C	0.69463	26.16538	1.30576
C	0.69857	27.59853	1.24881
C	6.82676	11.18474	1.63647
C	5.60030	10.50224	1.59627
C	4.37499	11.18915	1.60791
C	6.82435	12.62132	1.68136
C	5.59943	13.32950	1.68303
C	6.82630	15.47040	1.71160
C	3.15020	10.50481	1.59530
C	1.92545	11.19041	1.63621
C	4.37478	12.62397	1.65600
C	3.15059	13.33188	1.68247
C	5.60102	14.76131	1.70377
C	4.37534	15.46940	1.70535
C	6.82765	16.89936	1.68841
C	5.60215	17.60807	1.67151
C	6.82582	19.74532	1.54068
C	1.92654	12.62561	1.68090
C	3.15051	14.76150	1.70298
C	1.92481	15.47067	1.71102
C	4.37568	16.89960	1.69620
C	3.15022	17.60886	1.66574
C	5.60150	19.03619	1.59260
C	4.37519	19.74241	1.54246
C	6.82468	21.17288	1.46574
C	5.59845	21.87984	1.43111
C	6.82558	24.02301	1.48317
C	1.92486	16.89957	1.68409
C	3.14889	19.03488	1.58347
C	1.92520	19.74443	1.52655
C	4.37464	21.16867	1.44984
C	3.15125	21.88002	1.40398
C	5.59249	23.31157	1.46096
C	4.37343	24.00188	1.52155
C	6.82263	25.46289	1.46370
C	5.62291	26.17537	1.57482
C	6.82235	28.27901	1.27574
C	1.92501	21.17272	1.44078

C	3.15705	23.31179	1.42021
C	1.92395	24.02322	1.43487
C	3.12011	26.17481	1.53380
C	5.60240	27.59048	1.41051
C	4.37216	28.27865	1.38086
C	1.92236	25.46293	1.41693
C	3.14341	27.59156	1.38700
C	1.92426	28.27766	1.25089
C	4.36399	25.44847	1.96414
C	4.07725	16.95757	9.84165
C	4.39948	17.92571	10.80915
C	4.40644	19.63391	9.11710
C	4.07896	18.68349	8.14144
C	3.88654	17.36162	8.50650
C	4.56388	19.26762	10.45590
C	3.17035	20.92949	14.32295
C	3.81888	22.95666	13.20362
C	4.16787	23.51549	14.44175
C	4.04976	22.77185	15.61188
C	3.30497	21.65680	13.14316
C	3.97345	24.16451	5.65199
C	4.10475	25.32854	6.42195
C	4.30621	26.54542	5.74026
C	4.39904	26.59053	4.34666
C	4.29283	25.42254	3.57307
C	4.07466	24.22381	4.26376
C	4.10940	24.29361	8.71151
C	4.03145	23.53413	10.82598
C	4.37121	22.10562	9.14862
C	3.57750	21.44642	15.56641
C	5.22168	20.78420	18.05575
C	8.05380	10.50127	1.62717
C	8.05004	13.32899	1.71008
C	8.04983	14.75996	1.71962
C	8.05107	17.60907	1.65248
C	8.05120	19.03656	1.57886
C	8.04907	21.88435	1.44463
C	8.04531	23.31452	1.43086
C	8.04972	26.16592	1.33531
C	8.04843	27.60030	1.27290
C	9.27641	11.18802	1.66272
C	9.27597	12.62379	1.70487
C	9.27547	15.46984	1.71713
C	9.27584	16.89963	1.67636

C	9.27531	19.74663	1.53216
C	9.27516	21.17612	1.45927
C	9.27425	24.02412	1.38639
C	9.27214	25.45653	1.32972
C	9.27434	28.28607	1.22077
C	7.54858	21.34341	17.64881
C	7.85447	21.10627	18.99458
C	6.24865	21.18266	17.17435
C	6.84928	20.68860	19.87080
C	5.54779	20.52218	19.40235
C	6.62314	15.70079	11.12407
C	7.87004	15.48526	11.70782
C	8.09307	14.38377	12.54380
C	7.05691	13.48041	12.79244
C	5.81002	13.68732	12.21001
C	5.56610	14.80254	11.38487
N	4.24150	14.75665	10.83651
N	3.66654	15.62687	10.13643
N	3.85749	20.45295	17.76393
N	3.21780	20.65679	16.69798
N	3.95914	24.59607	10.02563
N	4.23264	22.25133	10.47058
N	4.32773	23.06273	8.22829
N	4.02448	25.33902	7.83292
O	3.90277	23.85628	12.13894
O	4.58944	20.90186	8.57643
H	0.70344	9.41517	1.58454
H	3.14764	9.41194	1.57917
H	5.59583	9.40866	1.57306
H	6.80720	29.36718	1.18717
H	4.37440	29.36496	1.26080
H	1.93452	29.36801	1.18519
H	3.91302	26.24145	8.29134
H	4.51845	17.62627	11.85179
H	3.94962	19.01515	7.11013
H	3.57427	16.61961	7.76901
H	4.81095	20.01861	11.20258
H	2.71767	19.93644	14.29997
H	4.52322	24.54612	14.46951
H	4.30325	23.22352	16.57218
H	2.99048	21.22324	12.19841
H	3.81477	23.20072	6.12650
H	4.40171	27.48407	6.29404
H	4.56707	27.56022	3.87130

H	3.98184	23.28246	3.72736
H	4.75114	20.16246	20.05733
H	4.98755	12.98432	12.35554
H	8.06259	9.41048	1.56610
H	9.27596	29.38055	1.20934
H	8.88001	21.22880	19.34947
H	6.03936	21.36193	16.12278
H	8.33647	21.65709	16.96084
H	7.08576	20.47101	20.91477
H	9.07826	14.22697	12.98742
H	7.22502	12.60727	13.42662
H	6.48082	16.55957	10.47214
H	8.68202	16.18893	11.51282

trans-RGO-bis-AZO** (1:72)

C	0.70231	10.49692	1.63923
C	6.82634	11.17290	1.63736
C	0.70135	13.32264	1.71169
C	5.60018	10.49011	1.59638
C	4.37542	11.17838	1.60738
C	6.82422	12.61013	1.67916
C	5.59953	13.31954	1.67685
C	0.70101	14.75238	1.71939
C	6.82635	15.46089	1.70514
C	0.70135	17.60030	1.63849
C	3.14986	10.49553	1.59823
C	1.92573	11.18194	1.64024
C	4.37562	12.61429	1.65086
C	3.15166	13.32297	1.67702
C	5.60137	14.75134	1.69632
C	4.37702	15.46128	1.69740
C	6.82823	16.89057	1.67879
C	5.60344	17.59966	1.66631
C	0.70026	19.02712	1.56299
C	6.82801	19.73684	1.53909
C	0.70357	21.87588	1.43000
C	1.92704	12.61717	1.67997
C	3.15191	14.75347	1.69630
C	1.92563	15.46214	1.70545
C	4.37742	16.89097	1.69022
C	3.15201	17.59983	1.66303
C	5.60363	19.02807	1.59486
C	4.37706	19.73438	1.55163

C	6.82692	21.16473	1.46818
C	5.60074	21.87113	1.44311
C	0.70832	23.30634	1.40556
C	6.82922	24.01489	1.46634
C	0.69889	26.15695	1.28924
C	1.92614	16.89098	1.67676
C	3.15065	19.02681	1.58904
C	1.92614	19.73563	1.52981
C	4.37696	21.16052	1.46763
C	3.15393	21.87125	1.42787
C	5.59569	23.30283	1.46573
C	4.37805	23.99465	1.53129
C	6.82743	25.45483	1.43130
C	5.62874	26.16940	1.53471
C	0.70290	27.58894	1.22216
C	6.82815	28.26923	1.21264
C	1.92733	21.16440	1.45298
C	3.16076	23.30335	1.44345
C	1.92780	24.01565	1.44294
C	3.12530	26.16848	1.51657
C	5.60817	27.58216	1.35298
C	4.37743	28.26859	1.31596
C	1.92708	25.45569	1.41116
C	3.14823	27.58261	1.34820
C	1.92844	28.26800	1.21466
C	4.37382	25.44904	1.94729
C	4.38726	17.31614	10.63819
C	4.82547	18.43981	11.35868
C	4.28658	19.86682	9.51510
C	3.85517	18.75488	8.77094
C	3.90136	17.48438	9.32483
C	4.78441	19.72088	10.81225
C	3.84159	21.86470	15.62128
C	3.23240	21.36189	14.46104
C	3.77454	23.37002	13.26474
C	4.37530	23.89764	14.41778
C	4.40816	23.15445	15.59053
C	3.17747	22.10685	13.28592
C	4.05321	24.25562	5.66678
C	4.13672	25.44614	6.40097
C	4.31908	26.64664	5.68676
C	4.41298	26.65284	4.29535
C	4.32688	25.46044	3.55603
C	4.15322	24.27580	4.27859

C	4.02269	24.48638	8.72752
C	3.88929	23.85358	10.87909
C	4.14739	22.31415	9.28507
C	3.93647	19.21081	18.81874
C	3.92827	18.41899	19.96197
C	4.22499	20.58603	18.92238
C	4.50074	20.34083	21.32170
C	4.51906	21.14054	20.17911
C	4.20223	18.98014	21.21739
C	4.46969	13.87208	12.89406
C	4.52192	12.67126	13.59111
C	4.17000	13.87446	11.51801
C	3.97454	11.45616	11.56763
C	3.91273	12.65934	10.86194
C	4.27949	11.45816	12.93154
C	8.05412	10.49084	1.63127
C	8.04934	13.31859	1.70989
C	8.05037	14.75025	1.71818
C	8.05230	17.60051	1.64008
C	9.27657	11.17873	1.66772
C	8.05296	19.02822	1.56738
C	8.05216	21.87619	1.44168
C	9.27648	12.61443	1.70684
C	9.27534	15.46094	1.71495
C	8.04897	23.30648	1.41961
C	8.05447	26.15693	1.30029
C	9.27666	16.89016	1.66659
C	9.27755	19.73793	1.52380
C	8.05381	27.59075	1.22687
C	9.27795	21.16756	1.45812
C	9.27837	24.01604	1.37675
C	9.27668	25.44787	1.31144
C	9.27952	28.27667	1.18470
N	3.87536	24.87030	10.02181
N	4.03003	22.54763	10.59334
N	4.15803	23.21746	8.30946
N	4.03280	25.49881	7.80801
N	3.82190	20.99659	16.73622
N	4.24856	21.48842	17.82676
N	4.47476	16.09911	11.34350
N	4.08943	15.05536	10.73005
O	3.75896	24.24299	12.17384
O	4.24372	21.05506	8.79380
H	3.96855	26.42045	8.23851

H	5.20221	18.28060	12.37133
H	3.49072	18.91974	7.75464
H	3.56440	16.61431	8.75990
H	5.11694	20.58416	11.38148
H	2.79003	20.36524	14.50041
H	4.81242	24.89668	14.36998
H	4.87212	23.54971	16.49460
H	2.70055	21.70176	12.39939
H	3.92184	23.31005	6.18124
H	4.39064	27.59936	6.21853
H	4.55778	27.61072	3.79239
H	4.09203	23.31623	3.77072
H	4.18667	18.35261	22.11127
H	3.72495	18.78807	17.83619
H	3.70841	17.35152	19.88170
H	4.72183	20.77829	22.29697
H	4.75189	22.20519	20.23800
H	4.32365	10.51838	13.48670
H	4.65341	14.82540	13.38926
H	4.75123	12.67630	14.65950
H	3.78143	10.51192	11.05409
H	3.67131	12.67815	9.79724
H	0.70542	9.40668	1.59386
H	3.14413	9.40245	1.58057
H	5.59619	9.39703	1.57258
H	6.81334	29.35698	1.11697
H	4.37680	29.35323	1.18417
H	1.93879	29.35825	1.13783
H	8.06346	9.39921	1.57212
H	9.28071	29.36929	1.16436

cis-RGO-*bis*-AZO* (1:90)

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C	0.68670	13.32222	1.66521
C	0.68828	14.74624	1.71199
C	0.69270	17.59827	1.73921
C	0.69206	19.01961	1.70293
C	0.69100	21.86831	1.55115
C	0.69760	23.29312	1.51597
C	0.68600	26.14768	1.49432
C	0.69041	27.58982	1.49835
C	6.83719	11.16507	1.61774
C	5.60663	10.48332	1.59706

C	4.37584	11.16535	1.62055
C	6.83784	12.60933	1.65638
C	5.60732	13.32089	1.68809
C	6.83944	15.45930	1.73217
C	3.14732	10.48250	1.60045
C	1.91883	11.16684	1.61752
C	4.37589	12.60991	1.67201
C	3.14688	13.32256	1.68854
C	5.60919	14.74593	1.72100
C	4.37977	15.45978	1.72581
C	6.84190	16.88022	1.73033
C	5.61189	17.59465	1.68377
C	6.84045	19.73155	1.62163
C	1.91737	12.61075	1.65693
C	3.14801	14.74798	1.71716
C	1.91638	15.46045	1.72448
C	4.38207	16.87916	1.69551
C	3.15153	17.59336	1.67059
C	5.60824	19.01383	1.60580
C	4.37956	19.72529	1.52295
C	6.84055	21.15231	1.54405
C	5.60926	21.86229	1.43865
C	6.84273	24.00296	1.55959
C	1.91957	16.88062	1.71818
C	3.15152	19.01300	1.59001
C	1.92024	19.73199	1.59698
C	4.37881	21.14683	1.42619
C	3.14792	21.86120	1.39766
C	5.60550	23.28688	1.45880
C	4.38160	23.98383	1.47370
C	6.84165	25.44071	1.56192
C	5.63706	26.15653	1.58632
C	6.85038	28.26550	1.40937
C	1.91555	21.15159	1.50237
C	3.15644	23.28784	1.40531
C	1.91826	24.00224	1.48640
C	3.12404	26.15406	1.53934
C	5.62137	27.57911	1.42872
C	4.38353	28.26347	1.34731
C	1.91954	25.43986	1.49365
C	3.14565	27.58031	1.40549
C	1.91930	28.26897	1.38865
C	4.37372	25.42219	1.93977
C	4.09685	16.96715	9.77654

C	4.43727	17.96253	10.70756
C	4.33822	19.64492	8.98780
C	4.01269	18.66201	8.04061
C	3.86613	17.34288	8.43942
C	4.55766	19.30070	10.32478
C	3.24463	20.94341	14.21548
C	3.83466	22.98202	13.09369
C	4.20146	23.55052	14.32073
C	4.10957	22.80759	15.49227
C	3.35202	21.67007	13.03582
C	3.97868	24.16579	5.59492
C	4.08235	25.34456	6.34265
C	4.28011	26.55983	5.66413
C	4.38416	26.59182	4.27601
C	4.29991	25.40559	3.52374
C	4.09951	24.20874	4.21540
C	4.07004	24.31778	8.61323
C	3.99052	23.54309	10.71523
C	4.29148	22.11903	9.02550
C	3.63776	21.48241	15.45250
C	5.23488	20.84808	17.97538
C	8.06842	10.48388	1.60653
C	8.06948	13.32134	1.66633
C	8.07112	14.74647	1.71631
C	8.07321	17.59632	1.74885
C	8.07086	19.01921	1.72246
C	8.06754	21.86850	1.59609
C	8.06575	23.29518	1.57863
C	8.07896	26.14538	1.54301
C	8.07826	27.58836	1.52479
C	11.75674	11.16500	1.60588
C	10.52648	10.48308	1.59851
C	9.29797	11.16755	1.60923
C	11.75679	12.60986	1.63237
C	10.52858	13.32091	1.65996
C	11.75975	15.45966	1.73765
C	9.29904	12.61129	1.63507
C	10.53131	14.74335	1.72365
C	9.30312	15.45893	1.74224
C	11.76335	16.88087	1.76112
C	10.53489	17.59793	1.77460
C	11.76259	19.73777	1.71565
C	9.30431	16.88120	1.76503
C	10.53337	19.02084	1.76039

C	9.30201	19.73692	1.73191
C	11.76212	21.15754	1.64750
C	10.53095	21.87140	1.64661
C	11.76255	24.00848	1.53547
C	9.29920	21.15740	1.66925
C	10.53279	23.29723	1.58279
C	9.30275	24.00801	1.57326
C	10.53366	26.14589	1.55289
C	11.76543	28.27279	1.59856
C	9.30514	25.43385	1.55451
C	10.53486	27.58853	1.60225
C	9.30576	28.27320	1.60626
C	11.76172	25.43422	1.52327
C	7.57351	21.43380	17.70119
C	7.82814	21.09647	19.03619
C	6.29356	21.30990	17.16095
C	6.79033	20.62631	19.84337
C	5.51125	20.50241	19.31207
C	6.62771	15.73866	11.20898
C	7.86241	15.50504	11.81279
C	8.07959	14.36173	12.59124
C	7.05151	13.43145	12.75813
C	5.81449	13.66096	12.16253
C	5.57470	14.81699	11.39307
N	4.25519	14.78573	10.83065
N	3.69226	15.64609	10.10889
N	3.87360	20.52523	17.66020
N	3.25561	20.71469	16.58284
N	3.92608	24.61194	9.92600
N	4.15812	22.25741	10.34848
N	4.27993	23.08887	8.12056
N	3.98700	25.36719	7.74503
O	3.88580	23.87283	12.02585
O	4.45336	20.91395	8.43173
H	0.69939	9.39142	1.59352
H	3.14340	9.39072	1.59133
H	5.60815	9.39017	1.57876
H	6.84902	29.35282	1.30589
H	4.38403	29.35237	1.24333
H	1.91900	29.36025	1.31109
H	3.89163	26.27455	8.19663
H	4.60133	17.69585	11.75201
H	3.84480	18.95724	7.00252
H	3.55690	16.57643	7.72632

H	4.81804	20.06308	11.05669
H	2.82736	19.93489	14.19814
H	4.54884	24.58511	14.34111
H	4.38818	23.26465	16.44234
H	3.04198	21.23791	12.08875
H	3.82548	23.21760	6.09644
H	4.35406	27.49105	6.23364
H	4.53469	27.55409	3.78017
H	4.03327	23.26616	3.67978
H	4.67812	20.11074	19.89901
H	4.99334	12.94706	12.25199
H	8.06949	9.39011	1.60442
H	10.52211	9.39121	1.57372
H	11.76527	29.36297	1.67078
H	9.30296	29.36507	1.68557
H	8.83753	21.18923	19.43919
H	6.13264	21.57333	16.11749
H	8.38835	21.80139	17.07236
H	6.97896	20.33786	20.87906
H	9.05252	14.19562	13.05639
H	7.21703	12.52104	13.33792
H	6.49251	16.63080	10.60172
H	8.66965	16.22774	11.67519

trans-RGO-bis-AZO* (1:90)

C	0.68737	10.46491	1.59832
C	6.84078	11.14887	1.61693
C	0.69095	13.30178	1.67215
C	5.61022	10.46583	1.59953
C	4.38096	11.15028	1.61362
C	6.84161	12.59157	1.65657
C	5.61178	13.30254	1.68746
C	0.69127	14.72777	1.71356
C	6.84116	15.44356	1.73491
C	0.69104	17.58401	1.73542
C	3.15238	10.46641	1.60144
C	1.91991	11.14705	1.61233
C	4.38084	12.59166	1.65987
C	3.14997	13.30140	1.68630
C	5.61118	14.72827	1.73128
C	4.38110	15.44266	1.74572
C	6.84088	16.86675	1.73551
C	5.61100	17.58191	1.70535

C	0.69207	19.00340	1.70279
C	6.84343	19.71656	1.63326
C	0.69543	21.85440	1.58519
C	1.92003	12.59017	1.65258
C	3.15073	14.72829	1.73246
C	1.92012	15.44429	1.73429
C	4.38119	16.86588	1.72826
C	3.15060	17.58166	1.70402
C	5.61076	19.00096	1.62992
C	4.38237	19.71081	1.56087
C	6.84512	21.13712	1.55550
C	5.61474	21.85062	1.45724
C	0.69900	23.28472	1.56868
C	6.84605	23.99589	1.57071
C	0.68515	26.14123	1.51893
C	1.91998	16.86676	1.73175
C	3.15163	19.00061	1.62351
C	1.92052	19.71774	1.61687
C	4.38365	21.13349	1.45670
C	3.15321	21.85001	1.43058
C	5.60819	23.27774	1.48065
C	4.38542	23.97454	1.50870
C	6.84624	25.43519	1.55579
C	5.64153	26.15014	1.57175
C	0.68837	27.58186	1.53580
C	6.84968	28.26592	1.44850
C	1.92056	21.13707	1.52605
C	3.16130	23.27860	1.44293
C	1.92119	23.99462	1.51965
C	4.38110	25.42280	1.94254
C	3.12247	26.15163	1.54962
C	5.62211	27.57516	1.44512
C	4.38277	28.26013	1.38809
C	1.92081	25.43415	1.51245
C	3.14311	27.57982	1.44029
C	1.91447	28.26603	1.44535
C	4.31077	17.30094	10.50805
C	4.70572	18.43810	11.22871
C	4.23538	19.83454	9.34694
C	3.86246	18.70498	8.59307
C	3.89956	17.44182	9.16640
C	4.68577	19.70457	10.66050
C	3.89946	21.95066	15.50889
C	3.37230	21.37880	14.34331

C	3.84405	23.38897	13.14828
C	4.36190	23.98665	14.31106
C	4.38614	23.27094	15.49484
C	3.32136	22.09447	13.15825
C	4.05029	24.23178	5.61146
C	4.12207	25.42903	6.33464
C	4.30399	26.63211	5.63232
C	4.40869	26.63050	4.24692
C	4.33413	25.43421	3.51669
C	4.16455	24.24725	4.22970
C	4.01428	24.46471	8.62494
C	3.93016	23.82347	10.75984
C	4.11484	22.28553	9.15080
C	3.94145	19.32285	18.62344
C	3.90199	18.49869	19.73822
C	4.24263	20.68753	18.78234
C	4.46774	20.37899	21.16749
C	4.51587	21.21187	20.05114
C	4.16027	19.02398	21.01351
C	4.46092	13.94784	12.86566
C	4.53084	12.77320	13.60326
C	4.15716	13.89274	11.49152
C	3.99579	11.47909	11.62406
C	3.91966	12.65510	10.87729
C	4.30147	11.53458	12.98632
C	8.06907	10.46340	1.60667
C	8.07202	13.30128	1.67413
C	11.75933	11.15040	1.60716
C	8.07084	14.72670	1.71539
C	8.07031	17.58325	1.74478
C	10.53241	10.46357	1.58895
C	9.30048	11.14428	1.61084
C	11.75957	12.59194	1.64427
C	10.52863	13.30226	1.66110
C	11.75957	15.44392	1.72408
C	8.07120	19.00350	1.71580
C	8.07102	21.85519	1.61798
C	9.29926	12.58953	1.64512
C	10.52889	14.72837	1.70340
C	9.29933	15.44504	1.72696
C	11.76004	16.86682	1.75166
C	10.52868	17.58339	1.77255
C	11.76127	19.71928	1.72356
C	8.06819	23.28461	1.61035

C	8.08038	26.14455	1.55675
C	9.29854	16.86840	1.75820
C	10.52962	19.00403	1.76755
C	9.29965	19.71992	1.73385
C	11.76396	21.14021	1.67894
C	10.53232	21.85706	1.69373
C	11.76106	24.00150	1.60999
C	8.07765	27.58511	1.55593
C	9.29997	21.14103	1.69438
C	10.53310	23.28671	1.65622
C	9.30320	24.00070	1.63529
C	11.76057	25.42932	1.57531
C	10.53186	26.14039	1.59843
C	11.76249	28.26827	1.63029
C	9.30377	25.42845	1.59987
C	10.53105	27.58435	1.62774
C	9.30229	28.26965	1.64231
N	3.90871	24.84458	9.91628
N	4.04160	22.51563	10.46382
N	4.11343	23.19808	8.18835
N	4.01927	25.48825	7.72901
N	3.87797	21.09990	16.61996
N	4.28554	21.60466	17.70897
N	4.37998	16.10996	11.25365
N	4.06831	15.03650	10.65381
O	3.84320	24.23152	12.04679
O	4.17247	21.02896	8.63910
H	3.97764	26.40873	8.16143
H	5.02970	18.29155	12.25953
H	3.55142	18.84476	7.55670
H	3.61126	16.55626	8.59539
H	4.99693	20.57536	11.22802
H	3.00492	20.35337	14.40431
H	4.73871	25.00937	14.25665
H	4.77989	23.70190	16.41815
H	2.90968	21.64472	12.25991
H	3.92615	23.29004	6.13441
H	4.37758	27.57949	6.17303
H	4.55329	27.58508	3.74602
H	4.11689	23.28865	3.72037
H	4.12247	18.36807	21.88586
H	3.74086	18.94834	17.61924
H	3.66692	17.43870	19.61812
H	4.66833	20.78535	22.16007

H	4.74976	22.27489	20.12715
H	4.36058	10.61601	13.57466
H	4.63806	14.92046	13.32532
H	4.76657	12.81664	14.66941
H	3.81667	10.51507	11.14394
H	3.68310	12.64167	9.81235
H	0.66939	9.37029	1.58497
H	3.16421	9.37397	1.58936
H	5.60689	9.37283	1.57337
H	6.84592	29.35802	1.37283
H	4.39039	29.35351	1.31879
H	1.90702	29.35719	1.39090
H	8.06115	9.36949	1.60056
H	10.54721	9.37028	1.55680
H	11.76777	29.36185	1.70037
H	9.30310	29.36141	1.70913